arXiv:cond-mat/9807414v1 [cond-mat.supr-con] 31 Jul 1998

Pairing Fluctuation Theory of Superconducting Properties in Underdoped to Overdoped Cuprates

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(February 1, 2008)

We propose a theoretical description of the superconducting state of under- to overdoped cuprates, based on the short coherence length of these materials and the associated strong pairing fluctuations. The calculated T_c and the zero temperature excitation gap $\Delta(0)$, as a function of hole concentration x, are in semi-quantitative agreement with experiment. Although the ratio $T_c/\Delta(0)$ has a strong x dependence, different from the universal BCS value, and $\Delta(T)$ deviates significantly from the BCS prediction, we obtain, quite remarkably, quasi-universal behavior, for the normalized superfluid density $\rho_s(T)/\rho_s(0)$ and the Josephson critical current $I_c(T)/I_c(0)$, as a function of T/T_c. While experiments on $\rho_s(T)$ are consistent with these results, future measurements on $I_c(T)$ are needed to test this prediction.

PACS numbers: 74.20.-z, 74.25.-q, 74.62.-c, 74.72.-h **cond-mat/9807414**

Pseudogap phenomena in the cuprates are of interest not only because of the associated unusual normal-state properties, but more importantly because of the constraints which these phenomena impose on the nature of the superconductivity and its associated high T_c. Moreover, this superconducting state presents an interesting challenge to theory: while the normal state is highly unconventional, the superconducting phase exhibits some features of traditional BCS superconductivity along with others which are strikingly different.

Thus far, there is no consensus on a theory of cuprate superconductivity. Scenarios which address the pseudogap state below T_c can be distinguished by the character of the excitations responsible for destroying superconductivity. In the theory of Lee and Wen [1], the destruction of the superconducting phase is associated with the excitation of the low-lying quasiparticles near the d-wave gap nodes. By contrast, Emery and Kivelson [2] argue that the destruction of the superconductivity is associated with low frequency, long wavelength phase fluctuations within a microscopically inhomogeneous model, based on one dimensional "stripes".

In the present paper, we present an alternative scenario in which, along with the quasiparticles of the usual BCS theory, there are additionally incoherent (but *not pre-formed*) pair excitations of finite momentum **q**, which assist in the destruction of superconductivity. This approach is based on a self-consistent treatment of the coupling of single particle and pair states. It represents a natural extension of BCS theory to the short coherence length (ξ) regime and provides a quantitative framework for addressing cuprate superconductivity. Here, we find a pronounced departure from BCS behavior in the underdoped limit which is continuously reduced with increasing hole concentration x. We derive a phase diagram for T_c and the zero temperature gap, $\Delta(0)$, as a function of x, which is in semi-quantitative agreement with (the anomalous) behavior observed in cuprate experiments, and we compute properties of the associated superconducting state such as the superfluid density ρ_s and Josephson critical current I_c. When these are plotted as $\rho_s(T)/\rho_s(0)$ and $I_c(T)/I_c(0)$, as a function of T/T_c, we deduce a quite remarkable, nearly universal behavior for the entire range of x.

As a simple model for the cuprate band structure, we consider a tight-binding, anisotropic dispersion $\epsilon_{\mathbf{k}} = 2\,t_\parallel(2 - \cos k_x - \cos k_y) + 2\ t_\perp(1-\cos k_\perp) - \mu$, where $t_\parallel$ ($t_\perp$) is the hopping integral for the in-plane (out-of-plane) motion and $t_\perp \ll t_\parallel$ [3]. We assume that the fermions interact via an effective pairing interaction with d-wave symmetry $V_{\mathbf{k},\mathbf{k}'} = -|g|\varphi_{\mathbf{k}}\varphi_{\mathbf{k}'}$ so that $\varphi_{\mathbf{k}} = \frac{1}{2}(\cos k_x - \cos k_y)$. The present approach is built on previous work [4–6] based on a particular diagrammatic theory, first introduced by Kadanoff and Martin [7], and subsequently extended by Patton [8]. This approach can be used to describe the widely discussed BCS to Bose-Einstein cross-over problem [9], which has been associated with small ξ. The "pairing approximation" of Refs. [7,8] leads to

$$\Sigma(K) = \sum_Q t(Q)\, G_o(Q-K)\, \varphi^2_{\mathbf{k}-\mathbf{q}/2}\ , \tag{1a}$$

$$g = [1 + g\chi(Q)]t(Q)\ , \tag{1b}$$

where $\Sigma(K)$ is the self-energy, $\chi(Q) = \sum_K G(K)\, G_o(Q-K)\varphi^2_{\mathbf{k}-\mathbf{q}/2}$ is the pair susceptibility. Equations (1), along with the number equation $n = 2\sum_K G(K)$, self-consistently determine both the Green's function $G(K)$ and the pair propagator, i.e., T-matrix $t(Q)$. We use a four-vector notation, e.g., $K \equiv (\boldsymbol{k}; i\omega)$, $\sum_K \equiv T\sum_{i\omega,\mathbf{k}}$ and $G_o(K) = (i\,\omega - \epsilon_{\mathbf{k}})^{-1}$. We now show that these equations yield a natural extension of BCS theory to include incoherent pairs (labeled by pg), along with the usual quasiparticles and superconducting condensate (labeled by sc).

We write the T-matrix and self-energy below T_c as $t(Q) = t_{sc}(Q) + t_{pg}(Q)$, and $\Sigma(K) = \Sigma_{sc}(K) + \Sigma_{pg}(K)$. The condensate contribution assumes the familiar BCS form $t_{sc}(Q) = -\delta(Q)\Delta^2_{sc}/T$, where Δ_{sc} is the superconducting gap parameter (and can be chosen to be real) and $\Sigma_{sc}(K) = \Delta^2_{sc}\,\varphi^2_{\mathbf{k}}/\,(i\omega + \epsilon_{\mathbf{k}})$. Inserting the above forms for the T-matrix into Eq. (1b), one obtains the gap equation $1 + g\chi(0) = 0$, as well as (for any non-zero Q), $t_{pg}(Q) = g/\,(1 + g\chi(Q))$. Note that because of the gap equation, $t_{pg}(Q)$ is highly peaked about the origin, with a divergence at $Q = 0$ [10].

As a consequence, in evaluating the associated contribution to the self-energy, the main contribution to the Q sum comes from this small Q divergent region so that $\Sigma_{pg}(K) \approx -G_o(-K)\Delta_{pg}^2\varphi_{\mathbf{k}}^2$, where we have defined the pseudogap parameter [11]

$$\Delta_{pg}^2 \equiv -\sum_Q t_{pg}(Q) = -\sum_Q \frac{g}{1+g\chi(Q)} \ . \tag{2a}$$

Thus, both Σ_{pg} and the total self-energy Σ can be well approximated by a BCS-like form, i.e., $\Sigma(K) \approx \Delta^2\, \varphi_{\mathbf{k}}^2/\,(i\omega_n + \epsilon_{\mathbf{k}})$, where $\Delta \equiv \sqrt{\Delta_{sc}^2 + \Delta_{pg}^2}$ is the magnitude of the total excitation gap, with the $\mathbf{k}$ dependence given by the d-wave function $\varphi_{\mathbf{k}}$. Within the above approximations, the gap and number equations reduce to

$$1 + g\sum_{\mathbf{k}} \frac{1-2f(E_{\mathbf{k}})}{2E_{\mathbf{k}}}\,\varphi_{\mathbf{k}}^2 = 0 \ , \tag{2b}$$

$$\sum_{\mathbf{k}} \left[1 - \frac{\epsilon_{\mathbf{k}}}{E_{\mathbf{k}}} + \frac{2\epsilon_{\mathbf{k}}}{E_{\mathbf{k}}}\, f(E_{\mathbf{k}})\right] = n \ , \tag{2c}$$

where the quasiparticle energy dispersion $E_{\mathbf{k}} = (\epsilon_{\mathbf{k}}^2 + \Delta^2\varphi_{\mathbf{k}}^2)^{1/2}$ contains the full excitation gap Δ.

The set of equations (2) can be used to determine the superconducting transition temperature T_c (where $\Delta_{sc} = 0$), and the temperature dependence of the various gap parameters. Eq. (2a) contains the physics of the pair excitations, or pseudogap. The remaining two Eqs. (2b) - (2c) are analogous to their BCS counterparts but with a finite (as a result of nonzero Δ_{pg}) excitation gap at T_c.

It should be stressed that physical quantities which characterize the superconducting state depend on the pair and particle excitations, as well as condensate in different ways. The superfluid density can be written in terms of the London penetration depth as $\rho_{s,ab}(T)/\rho_{s,ab}(0) = [\lambda_{ab}(0)/\lambda_{ab}(T)]^2$, where

$$\lambda_{ab}^{-2} = \frac{4\pi e^2\Delta_{sc}^2}{c^2}\sum_{\mathbf{k}} \frac{\varphi_{\mathbf{k}}}{E_{\mathbf{k}}^2}\left[\frac{1-2f(E_{\mathbf{k}})}{2E_{\mathbf{k}}} + f'(E_{\mathbf{k}})\right] \times \left[\varphi_{\mathbf{k}}\left(\frac{\partial\epsilon_{\mathbf{k}}}{\partial\mathbf{k}_\parallel}\right)^2 - \epsilon_{\mathbf{k}}\frac{\partial\epsilon_{\mathbf{k}}}{\partial\mathbf{k}}\cdot\frac{\partial\varphi_{\mathbf{k}}}{\partial\mathbf{k}}\right] \ . \tag{3}$$

During the calculation special attention should be paid to lattice effects [12] and to the vertex correction (associated with the pseudogap self-energy) which enforces gauge invariance via the generalized Ward identity. This identity insures that $\rho_s \propto \Delta_{sc}^2$ and it vanishes identically at and above T_c. The prefactor $\Delta_{sc}^2 = \Delta^2 - \Delta_{pg}^2$ in Eq. (3) indicates that pairs (in addition to quasiparticles) serve to reduce the superfluid density.

In a related fashion, we address c-axis Josephson tunneling between two identical high T_c superconductors. This situation is relevant to both break junction experiments [13] and to intrinsic Josephson tunneling [14] as well. An expression for the Josephson critical current [15] can be derived under the presumption that the tunneling matrix element

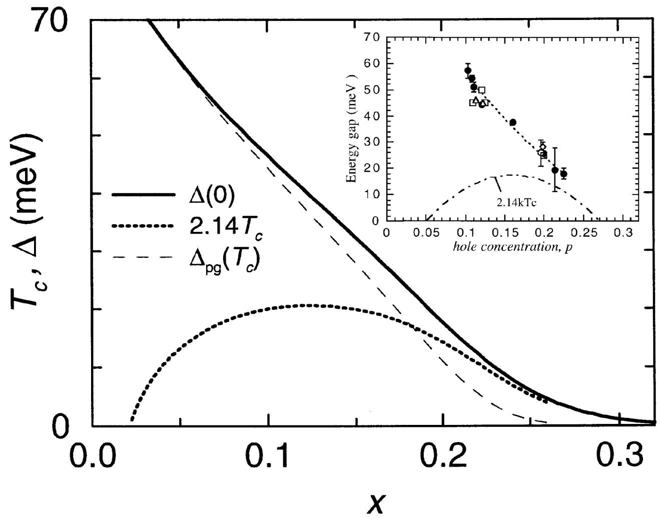

FIG. 1. Phase diagram showing $\Delta(0)$ and T_c as well as $\Delta_{pg}(T_c)$. The inset shows experimental results from Ref. [13].

$|T_{\mathbf{kp}}|^2 = |T_0|^2\,\delta_{\mathbf{k}_\parallel\mathbf{p}_\parallel} + |T_1|^2$, where only the first (coherent) term contributes for a d-wave order parameter,

$$I_c = 2e|T_0|^2\Delta_{sc}^2\sum_{\mathbf{kp}}\delta_{\mathbf{k}_\parallel\mathbf{p}_\parallel}\frac{\varphi_{\mathbf{k}}\varphi_{\mathbf{p}}}{E_{\mathbf{k}}E_{\mathbf{p}}} \times \left[\frac{1-f(E_{\mathbf{k}})-f(E_{\mathbf{p}})}{E_{\mathbf{k}}+E_{\mathbf{p}}} + \frac{f(E_{\mathbf{k}})-f(E_{\mathbf{p}})}{E_{\mathbf{k}}-E_{\mathbf{p}}}\right] \ . \tag{4}$$

Equation (4), like Eq. (3), differs from the usual BCS form (as well as that assumed by Lee and Wen [1,16]) in that the prefactor Δ_{sc}^2 is no longer the total excitation gap Δ^2.

The remainder of this paper is directed towards understanding three experimental characteristics of the cuprates: (i) the phase diagram, (ii) the superfluid density and (iii) the Josephson critical current.

(i) In order to generate physically realistic values of the various energy scales, we make two assumptions: (1) We take g as doping-independent (which is not unreasonable in the absence of any more detailed information about the pairing mechanism) and (2) incorporate the effect of the Mott transition at half filling, by introducing an x-dependence into the in-plane hopping matrix elements $t_\parallel$, as would be expected in the limit of strong on-site Coulomb interactions in a Hubbard model [17]. Thus the hopping matrix element is renormalized as $t_\parallel(x) \approx t_0(1-n) = t_0 x$, where t_0 is the matrix element in the absence of Coulomb effects. This x dependent energy scale is consistent with the requirement that the plasma frequency vanish at $x = 0$. These assumptions leave us with one free parameter $-g/4t_0$, for which we assign the value 0.15 to optimize the overall fit of the phase diagram to experiment. We take $t_\perp/t_\parallel \approx 0.01$ [18], and $t_0 \approx 0.6$ eV, which is reasonably consistent with experimentally based estimates [19].

The results for T_c, obtained from Eqs. (2), as a function of x are plotted in Fig. 1. Also indicated is the corresponding zero temperature excitation gap $\Delta(0)$ as well as the pseudogap Δ_{pg} at T_c. These three quantities provide us, for use in

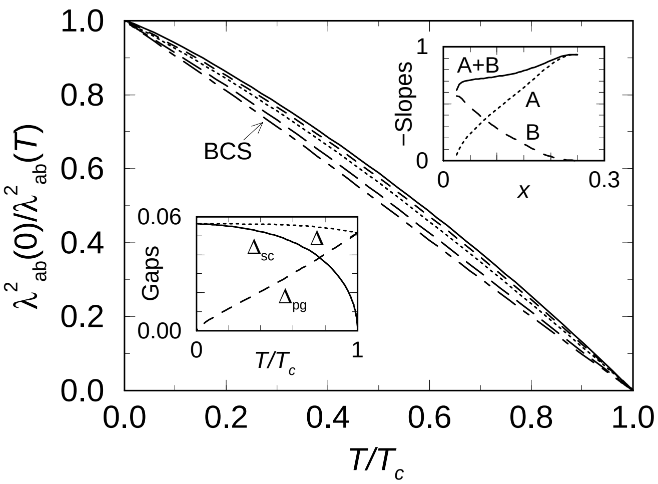

FIG. 2. Temperature dependence of the ab-plane inverse squared penetration depth. **Main figure**: from bottom to top are plotted for $x = 0.25$ (BCS limit, dot-dashed line), 0.2 (long-dashed), 0.155 (dotted), 0.125 (dashed) and 0.05 (solid line). **Lower inset**: energy gaps as a function of T/T_c for $x = 0.125$. **Upper inset**: (A) the slope given by the low temperature expansion assuming a constant $\Delta_{sc}(T) = \Delta(0)$; (B) the ratio $\frac{\Delta^2_{sc}(T)}{\Delta^2(0)} / \frac{T}{T_c}$ at $T/T_c = 0.2$; and (A+B) the sum of two contributions.

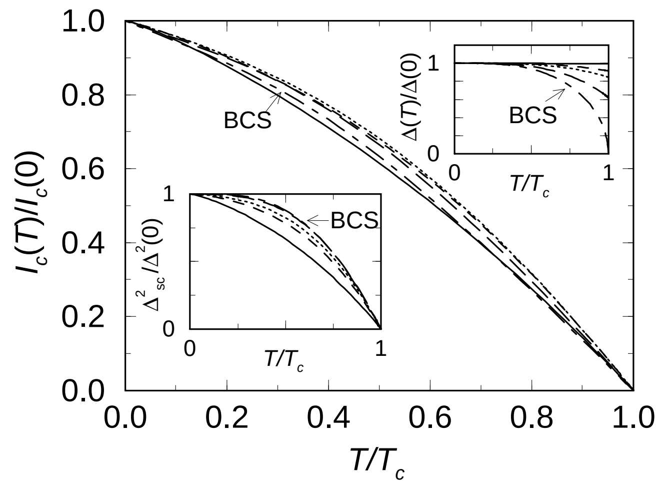

FIG. 3. Temperature dependence of c-axis Josephson critical current for doping concentrations corresponding to the legends in Fig. 2 (main figure). The variation of Δ^2_{sc} and Δ as a function of T/T_c are plotted in the insets for the corresponding values of x.

subsequent calculations, with energy scales which are in reasonable agreement with the data of Ref. [13], shown in the inset. The temperature dependences of the energy gaps in Fig. 1 are shown as the lower inset to Fig. 2, for a slightly underdoped case with $x = 0.125$. The relative size of $\Delta_{pg}(T_c)$, compared to $\Delta(0)$, increases with decreasing x. In the highly overdoped limit this ratio approaches zero, and the BCS limit is recovered. This inset illustrates the general behavior as a function of T/T_c: the excitation gap Δ is, generally, finite at T_c , the superconducting gap Δ_{sc} is established at and below T_c, while the pseudogap Δ_{pg} decreases to zero as T is reduced from T_c to 0. This last observation is consistent with general expectations for $\Delta^2_{pg} \approx \left\langle|\Delta|^2\right\rangle - |\Delta_{sc}|^2$ [11].

It is important to stress, that our subsequent results for the superfluid density and Josephson current, need not be viewed as contingent on the detailed x-dependence used to derive the phase diagram. One can approach the calculations of these quantities by taking $T_c(x)$ and the various gap parameters (shown in the inset) as phenomenological inputs, within the context of the present formalism.

(ii) The superfluid density (normalized to its $T = 0$ value), given by Eq. (3), is plotted in Fig. 2 as a function of T/T_c for several representative values of x, ranging from the highly over- to highly underdoped regimes. These plots clearly indicate a "quasi-universal" behavior with respect to x: $\rho_s(T)/\rho_s(0)$ *vs.* T/T_c depends only slightly on x. Moreover, the shape of these curves follows closely that of the weak-coupling BCS theory. The, albeit, small variation with x is systematic, with the lowest value of x corresponding to the top curve. Recent experiments provide some preliminary evidence for this universal behavior [20,21]. However, a firm confirmation requires further experiments on a wider range of hole concentrations, from extreme under- to overdoped samples [22]. This universal behavior appears surprising at first sight [1,16] because of the strong x dependence in the ratio $T_c/\Delta(0)$ (see Fig. 1). It should be noted that universality would *not* persist if $\rho_s(T)/\rho_s(0)$ were plotted in terms of $T/\Delta(0)$. The nontrivial origin of this effect has a simple explanation within the present theory. At low to intermediate temperatures, it follows from Eq. (3) that $\lambda^2_{ab}(0)/\lambda^2_{ab}(T) = \left(\Delta^2_{sc}(T)/\Delta^2(0)\right)\left(1 - AT/T_c + \mathcal{O}\left[(T/T_c)^2\right]\right) \approx 1 - [A + B(T)]\,(T/T_c)$, where terms of order $(T/T_c)^2$ and higher have been neglected. Here $A = 32\sqrt{2}\ln 2\left(e^2\lambda^2_{ab}(0)/c^2\right) t_\parallel \times (T_c/\Delta(0))$ represents the standard contribution to the linear T dependence of $\rho_s(T)$. The new term $B(T) = (T_c/T)\,\Delta^2_{pg}(T)/\Delta^2(0)$ derives from the pseudogap contribution and has a weaker than linear T dependence (as can be inferred from the lower inset in Fig. 3) [23]. For the purposes of illustration, these two terms are plotted in the upper inset of Fig. 2 at $T/T_c = 0.2$. Note that the effective (negative) "slope" $A + B$ is relatively x independent over the physical range of hole concentrations. Physically, the terms A and B are associated with two compensating contributions, arising from the quasiparticle and pair excitations, respectively, so that quasi-universal behavior results at low T. It can be shown that the same compensating effect obtains all the way to T_c, as is exhibited in Fig. 2. Thus, the destruction of the superconducting state comes predominantly from pair excitations at low x, and quasiparticle excitations at high x.

(iii) Finally, as plotted in Fig. 3, we obtain from Eq. (4), similarly, unexpected quasi-universal behavior for the normalized c-axis Josephson critical current for the same wide range of x as in Fig. 2. This behavior is in contrast to the strongly x dependent quasiparticle tunneling characteristics which can be inferred from the temperature dependent excitation gap plotted in the upper inset of Fig. 3. The origin of this univer-

sality is essentially the same as that for ρ_s, deriving from two compensating contributions. At this time, there do not appear to be detailed studies of $I_c(T)$ as a function of x, although future measurements will, ultimately, be able to determine this quantity. In these future experiments the quasiparticle tunneling characteristics should be simultaneously measured, along with $I_c(T)$, so that direct comparison can be made to the excitation gap; in this way, the predictions indicated in Fig. 3 and its upper inset can be tested. Indications, thus far [13,24], are that this tunneling excitation gap coincides rather well with values obtained from photoemission data (see Fig. 1).

In summary, in this paper we have proposed a scenario for the superconducting state of the cuprates. This state evolves continuously with hole doping x, exhibiting unusual features at low x (associated with a large excitation gap at T_c) and manifesting the more conventional features of BCS theory at high x. In this scenario the pseudogap state is associated with pair excitations, which act in concert with the usual quasiparticles. Despite the fact that the underdoped cuprates exhibit features inconsistent with BCS theory ($T_c/\Delta(0)$ is strongly x dependent and Δ is finite at and above T_c) we deduce an interesting quasi-universality of the normalized ρ_s and I_c as a function of T/T_c. In these plots the over- and under-doped systems essentially appear indistinguishable. Current experiments lend support to this universality in ρ_s, although a wider range of hole concentrations will need to be addressed, along with future systematic measurements of I_c.

We would like to thank D. A. Bonn, P. Guptasarma, W. N. Hardy, M. Norman and J. F. Zasadzinski for useful discussions. We gratefully acknowledge the hospitality of the Aspen Center for Physics, where part of this work was completed. This research was supported in part by the Science and Technology Center for Superconductivity funded by the National Science Foundation under award No. DMR 91-20000.

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[11] As expected, Δ_{pg} is related to the fluctuations of the pair operator, $\hat{\Delta}_{\mathbf{q}} \equiv g\sum_{\mathbf{k}}\varphi_{\mathbf{k}} c_{-\mathbf{k}+\mathbf{q}/2\downarrow} c_{\mathbf{k}+\mathbf{q}/2\uparrow}$, about its mean field value $|\Delta_{sc}| = |\langle\hat{\Delta}_{\mathbf{q}=0}\rangle|$. Indeed, $\langle|\Delta|^2\rangle \equiv \sum_{\mathbf{q}}\langle\hat{\Delta}_{\mathbf{q}}\hat{\Delta}^\dagger_{\mathbf{q}}\rangle = g^2\sum_{K,K'}\varphi_{\mathbf{k}}\varphi_{\mathbf{k}'} C_2(K,K')$, where the irreducible two-particle correlation function $C_2(K,K') = -\sum_Q t(Q)\,A(K;Q)\,A(K';Q)$, with $A(K;Q) = G_o(-K+Q/2)\,G(K+Q/2)\,\varphi_{\mathbf{k}}$, in the absence of off-diagonal-long-range-order cannot be factorized in the variables K and K'. This expression for C_2 defines the T-matrix $t(Q)$. The combination of bare and fully dressed Green's functions enter $A(K;Q)$; for $t(Q) = t_{sc}(Q)$, one recovers the Gor'kov factorization $C_2(K,K') = F(K)\,F^*(K')$, where $F(K) = \Delta_{sc}\varphi_{\mathbf{k}} G_o(-K) G(K)$ is the Gor'kov anomalous Green's function. Thus, by taking $t(Q) = t_{sc}(Q) + t_{pg}(Q)$, recalling the definition of the pair susceptibility $\chi(Q)$, and using the expression for the gap equation, one has $\left\langle|\Delta|^2\right\rangle = -\sum_Q t(Q)\,[g\chi(Q)]^2 = |\Delta_{sc}|^2 + \left(-\sum_Q t_{pg}(Q)[g\chi(Q)]^2\right) \approx |\Delta_{sc}|^2 + \Delta^2_{pg}$, where we have exploited once again the fact that, for $T \le T_c$, $t_{pg}(Q)$ is highly peaked around $Q = 0$.

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